6«alpha»-Hydroxy-4-Chloro-1,2,dehydro-17«alpha»-tris-TMS

Inchi: InChI=1S/C29H51ClO3Si3/c1-27-16-15-23(31-34(4,5)6)26(30)25(27)24(32-35(7,8)9)19-2

InchiKey: RJRDWQNBTOPZNE-UHFFFAOYSA-N

Formula: C29H51ClO3Si3

SMILES: CC12C=CC(O[Si](C)(C)C)=C(Cl)C1=C(O[Si](C)(C)C)CC1C2CCC2(C)C1CCC2(C)O[Si](C

Mol. weight [g/mol]: 567.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Crippen Method
logp	9.426		Crippen Method
rinpol	3018.00		NIST Webbook
rinpol	3018.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U412281&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices